



IN PARTNERSHIP WITH:  
**Ecole des Ponts ParisTech**

Activity Report 2013

## **Project-Team MICMAC**

Methods and engineering of multiscale  
computing from atom to continuum

IN COLLABORATION WITH: Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique  
(CERMICS)

RESEARCH CENTER  
**Paris - Rocquencourt**

THEME  
**Computational models and simulation**



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# Project-Team MICMAC

**Keywords:** Scientific Computation, Model Coupling, Quantum Physics, Statistical Physics, Multiscale Models, Homogenization

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## 1. Members

### Research Scientists

Claude Le Bris [Team leader, ENPC, until Dec 2013, HdR]  
Sébastien Boyaval [ENPC, until Dec 2013]  
Eric Cancès [ENPC, until Dec 2013, HdR]  
Ismaila Dabo [ENPC, until Aug 2013]  
Virginie Ehrlacher [ENPC, until Dec 2013]  
Frédéric Legoll [ENPC, until Dec 2013, HdR]  
Tony Lelièvre [ENPC, until Dec 2013, HdR]  
Mathias Rousset [Inria, Researcher, until Dec 2013]  
Gabriel Stoltz [ENPC, until Dec 2013, HdR]

### Faculty Member

Francis Nier [Univ. Rennes I, Professor, until Aug 2013]

### PhD Students

David Benoit [Univ. Paris Est, until Dec 2013]  
David Gontier [Univ. Paris Est, until Dec 2013]  
Salma Lahbabi [CNRS, until Sep 2013]  
François Madiot [Univ. Paris Est, from Oct 2013]  
William Minvielle [Univ. Paris Est, until Dec 2013]

### Post-Doctoral Fellows

Charles-Edouard Bréhier [Inria, from Sep 2013, until Dec 2013]  
Davide Bianco [Univ. Paris Est, from Jun 2013, until Dec 2013]

### Other

Marine Meyer [Inria, Administrative assistant, TR]

## 2. Overall Objectives

### 2.1. Overall Objectives

The MICMAC project-team has been created jointly by the Ecole des Ponts ParisTech (ENPC) and Inria in October 2002. It is hosted by the CERMICS laboratory (Centre d'Enseignement et de Recherches en Mathématiques et Calcul Scientifique) at ENPC. The permanent research scientists of the project-team have positions at CERMICS and at two other laboratories of Ecole des Ponts: Institut Navier and Laboratoire Saint-Venant. The scientific focus of the project-team is to analyze and improve the numerical schemes used in the simulation of computational chemistry at the microscopic level and to create simulations coupling this microscopic scale with meso- or macroscopic scales (possibly using parallel algorithms). Over the years, the project-team has accumulated an increasingly solid expertise on such topics, which are traditionally not well known by the community in applied mathematics and scientific computing. One of the major achievements of the project-team is to have created a corpus of literature, authoring books and research monographs on the subject [1], [2], [3], [5], [6] that other scientists may consult in order to enter the field.

## 3. Research Program

### 3.1. Research Program

Quantum Chemistry aims at understanding the properties of matter through the modeling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström ( $10^{-10}$  meters), and the size of the nucleus embedded in it is  $10^{-15}$  meters; the typical vibration period of a molecular bond is the femtosecond ( $10^{-15}$  seconds), and the characteristic relaxation time for an electron is  $10^{-18}$  seconds. Consequently, Quantum Chemistry calculations concern very short time (say  $10^{-12}$  seconds) behaviors of very small size (say  $10^{-27}$  m<sup>3</sup>) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability minerals have to naturally split along crystal surfaces (e.g. mica yields to thin flakes) is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time dependent form or in its time independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its  $L^2$  norm is set to one.

The time dependent equation is a first order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical

simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of  $L^2(\mathbb{R}^d)$ , with  $d = 3(M + N)$ ,  $M$  and  $N$  respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter  $d$  is already 39 for a single water molecule and rapidly reaches  $10^6$  for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is  $10^4$  times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on  $L^2(\mathbb{R}^3)$ . The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales. Such problems are described in the following sections.

## 4. Application Domains

### 4.1. Electronic structure of large systems

As the size of the systems one wants to study increases, more efficient numerical techniques need to be resorted to. In computational chemistry, the typical scaling law for the complexity of computations with respect to the size of the system under study is  $N^3$ ,  $N$  being for instance the number of electrons. The Holy Grail in this respect is to reach a linear scaling, so as to make possible simulations of systems of practical interest in biology or material science. Efforts in this direction must address a large variety of questions such as

- how can one improve the nonlinear iterations that are the basis of any *ab initio* models for computational chemistry?
- how can one more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?
- how can one design a sufficiently small variational space, whose dimension is kept limited while the size of the system increases?

An alternative strategy to reduce the complexity of *ab initio* computations is to try to couple different models at different scales. Such a mixed strategy can be either a sequential one or a parallel one, in the sense that

- in the former, the results of the model at the lower scale are simply used to evaluate some parameters that are inserted in the model for the larger scale: one example is the parameterized classical molecular dynamics, which makes use of force fields that are fitted to calculations at the quantum level;
- while in the latter, the model at the lower scale is concurrently coupled to the model at the larger scale: an instance of such a strategy is the so called QM/MM coupling (standing for Quantum Mechanics/Molecular Mechanics coupling) where some part of the system (typically the reactive site of a protein) is modeled with quantum models, that therefore accounts for the change in the electronic structure and for the modification of chemical bonds, while the rest of the system (typically the inert part of a protein) is coarse grained and more crudely modeled by classical mechanics.

The coupling of different scales can even go up to the macroscopic scale, with methods that couple a microscopic description of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

## 4.2. Computational Statistical Mechanics

The orders of magnitude used in the microscopic description of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number  $N_A \sim 10^{23}$ , the typical distances are expressed in Å ( $10^{-10}$  m), the energies are of the order of  $k_B T \simeq 4 \times 10^{-21}$  J at room temperature, and the typical times are of the order of  $10^{-15}$  s when the proton mass is the reference mass.

To give some insight into such a large number of particles contained in a macroscopic sample, it is helpful to compute the number of moles of water on earth. Recall that one mole of water corresponds to 18 mL, so that a standard glass of water contains roughly 10 moles, and a typical bathtub contains  $10^5$  mol. On the other hand, there are approximately  $1.3 \times 10^{18}$  m<sup>3</sup> of water in the oceans, *i.e.*  $7.2 \times 10^{22}$  mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating  $N_A$  atoms and performing  $O(10^{15})$  time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of 0.1  $\mu$ s.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of  $N$  particles correctly approximate the macroscopic property, formally obtained in the thermodynamic limit  $N \rightarrow +\infty$  (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

Despite its intrinsic limitations on spatial and timescales, molecular simulation has been used and developed over the past 50 years, and its number of users keeps increasing. As we understand it, it has two major aims nowadays.

First, it can be used as a *numerical microscope*, which allows us to perform “computer” experiments. This was the initial motivation for simulations at the microscopic level: physical theories were tested on computers. This use of molecular simulation is particularly clear in its historic development, which was triggered and sustained by the physics of simple liquids. Indeed, there was no good analytical theory for these systems, and the observation of computer trajectories was very helpful to guide the physicists' intuition about what was happening in the system, for instance the mechanisms leading to molecular diffusion. In particular, the pioneering works on Monte-Carlo methods by Metropolis et al, and the first molecular dynamics simulation of Alder and Wainwright were performed because of such motivations. Today, understanding the behavior of matter at the microscopic level can still be difficult from an experimental viewpoint (because of the high resolution required, both in time and in space), or because we simply do not know what to look for! Numerical simulations are then a valuable tool to test some ideas or obtain some data to process and analyze in order to help assessing experimental setups. This is particularly true for current nanoscale systems.

Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative answers. Sometimes, these properties are accessible through experiments, but in some cases only numerical computations are possible since experiments may be unfeasible or too costly (for instance, when high pressure or large temperature regimes are considered, or when studying materials not yet synthesized). More generally, molecular simulation is a tool to explore the links between the microscopic and macroscopic properties of a



material, allowing one to address modelling questions such as “Which microscopic ingredients are necessary (and which are not) to observe a given macroscopic behavior?”

### 4.3. Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on how to couple models written at the atomistic scale, with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

The following observation motivates the idea of coupling atomistic and continuum description of materials. In many situations of interest (crack propagation, presence of defects in the atomistic lattice, ...), using a model based on continuum mechanics is difficult. Indeed, such a model is based on a macroscopic constitutive law, the derivation of which requires a deep qualitative and quantitative understanding of the physical and mechanical properties of the solid under consideration. For many solids, reaching such an understanding is a challenge, as loads they are submitted to become larger and more diverse, and as experimental observations helping designing such models are not always possible (think of materials used in the nuclear industry). Using an atomistic model in the whole domain is not possible either, due to its prohibitive computational cost. Recall indeed that a macroscopic sample of matter contains a number of atoms on the order of  $10^{23}$ . However, it turns out that, in many situations of interest, the deformation that we are after is not smooth in *only a small part* of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them, in a domain decomposition spirit. In most of the domain, the deformation is expected to be smooth, and reliable continuum mechanics models are then available. In the rest of the domain, the expected deformation is singular, one needs an atomistic model to describe it properly, the cost of which remains however limited as this region is small.

From a mathematical viewpoint, the question is to couple a discrete model with a model described by PDEs. This raises many questions, both from the theoretical and numerical viewpoints:

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to be a good description of the materials;
- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

More generally, the presence of numerous length-scales in material science problems represents a challenge for numerical simulation, especially when some *randomness* is assumed on the materials. It can take various forms, and includes defects in crystals, thermal fluctuations, and impurities or heterogeneities in continuous media. Standard methods available in the literature to handle such problems often lead to very costly computations. Our goal is to develop numerical methods that are more affordable. Because we cannot embrace all difficulties at once, we focus on a simple case, where the fine scale and the coarse-scale models can be written similarly, in the form of a simple elliptic partial differential equation in divergence form. The fine scale model includes heterogeneities at a small scale, a situation which is formalized by the fact that the coefficients in the fine scale model vary on a small length scale. After homogenization, this model yields an effective, macroscopic model, which includes no small scale. In many cases, a sound theoretical groundwork exists for such homogenization results. We consider mostly the setting of stochastic homogenization of linear, scalar, second order elliptic PDEs, where analytical formulas for the effective properties are known. The difficulty stems from the fact that they generally lead to prohibitively costly computations. For such a case, simple from the theoretical viewpoint, our aim is to focus on different practical computational approaches to speed-up the computations. One possibility, among others, is to look for specific random materials, relevant from the practical viewpoint, and for which a dedicated approach can be proposed, that is less expensive than the general approach.

## 5. New Results

### 5.1. Electronic structure calculations

**Participants:** Eric Cancès, Ismaila Dabo, Virginie Ehrlicher, David Gontier, Salma Lahbabi, Claude Le Bris, Gabriel Stoltz.

In electronic structure calculation as in most of our scientific endeavours, we pursue a twofold goal: placing the models on a sound mathematical grounding, and improving the numerical approaches.

E. Cancès and S. Lahbabi have addressed issues related to the modeling and simulation of defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. In collaboration with M. Lewin (CNRS, Cergy), E. Cancès and A. Deleurence have proposed in 2008 a new model for describing the electronic structure of a crystal in the presence of a local defect. This model is based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics (QED) in the presence of an external electrostatic field. The justification of this model is obtained using a thermodynamic limit of Kohn-Sham type models. In collaboration with M. Lewin, E. Cancès and S. Lahbabi have introduced a functional setting for mean-field electronic structure models of Hartree-Fock or Kohn-Sham types for disordered quantum systems, and used these tools to study the reduced Hartree-Fock model for a disordered crystal where the nuclei are classical particles whose positions and charges are random.

D. Gontier has obtained a complete, explicit, characterization of the set of spin-polarized densities for finite molecular systems. This problem was left open in the pionnering work of von Barth and Hedin setting up the Kohn-Sham density functional theory for magnetic compounds.

On the numerical side, E. Cancès, L. He (ENPC), Y. Maday (University Paris 6) and R. Chakir (IFSTTAR) have designed and analyzed a two-grid methods for nonlinear elliptic eigenvalue problems, which can be applied, in particular, to the Kohn-Sham model. Some numerical tests demonstrating the interest of the approach have been performed with the Abinit software.

Implicit solvation models aims at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous media accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. A collaboration with F. Lipparini (Paris 6), B. Mennucci (Department of Chemistry, University of Pisa) and J.-P. Picquemail (Paris 6) is in progress to implement this algorithm in widely used computational softwares (Gaussian and Tinker), and to extend this method to other implicit solvation models.

Claude Le Bris, in collaboration with Pierre Rouchon (Ecole des Mines de Paris), has pursued the study of a new efficient numerical approach, based on a model reduction technique, to simulate high dimensional Lindblad type equations at play in the modelling of open quantum systems. The specific case under consideration is that of oscillation revivals of a set of atoms interacting resonantly with a slightly damped coherent quantized field of photons. The approach may be employed for other similar equations. Current work is directed towards other numerical challenges for this type of problems.

### 5.2. Computational Statistical Physics

**Participants:** Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Francis Nier, Mathias Rousset, Gabriel Stoltz.

#### 5.2.1. Free Energy calculations

For large molecular systems, the information of the whole configuration space may be summarized in a few coordinates of interest, called reaction coordinates. An important problem in chemistry or biology is to compute the effective energy felt by those reaction coordinates, called free energy.

In [39], T. Lelièvre and G. Stoltz, in collaboration with physicists from CEA Saclay (especially, M. Athenes) studied a new adaptive technique of ABF type to compute on-the-fly the free energy of a system, without evaluating the second derivatives of the reaction coordinate. The method uses a Bayesian reinterpretation of an extended system where the reaction coordinate is considered as an additional variable.

In [44], G. Fort (Telecom Paris), B. Jourdain (CERMICS), E. Kuhn (INRA), T. Lelièvre and G. Stoltz have studied the efficiency of the Wang-Landau algorithm, building on a previous study where they proved the convergence of this method. The aim was to obtain precise estimates of the exit times out of metastable states. This was done in two ways: a theoretical study in the simplest possible metastable situation, a system with three states; and a numerical study in a more realistic situation (a two-dimensional double well potential).

### 5.2.2. *Sampling trajectories*

There exist a lot of methods to sample efficiently Boltzmann-Gibbs distributions. The situation is much more intricate as far as the sampling of trajectories (and especially metastable trajectories) is concerned.

Recently, the quasi stationary distribution has been identified by the team as a good mathematical tool to analyze metastable trajectories, and to make a link between a continuous state space dynamics (Langevin dynamics) and a discrete state space dynamics (kinetic Monte Carlo models), see for example lelievre-13. This perspective can also be used to analyze accelerated dynamics techniques which have been proposed by A. Voter in the late nineties, to simulate very efficiently the state-to-state dynamics associated with metastable trajectories. For example, in [33], T. Lelièvre with D. Aristoff (University of Minnesota) propose a mathematical analysis of the Temperature Accelerated Dynamics. In [49], T. Lelièvre and F. Nier have studied the quasi-stationary distribution for an overdamped Langevin process in a bounded domain. In the small temperature limit and by making the connection with boundary Witten Laplacians, they are able to accurately compute the spatial exit law along the boundary and non perturbative accurate formulas when the potential is changed inside the domain. This gives some insight into the foundations of the hyperdynamics method.

Finally, following a numerical observation in a previous work on the sampling of reactive trajectories by a multilevel splitting algorithm, F. Cérou (Inria Rennes), A. Guyader (Inria Rennes), T. Lelièvre and F. Malrieu (Université de Rennes) study theoretically in [19] the distribution of the lengths of these trajectories, using large deviation techniques.

### 5.2.3. *Nonequilibrium systems*

Let us also mention that the article [22] on a derivation of a Langevin-type dynamics for a heavy particle in a non-zero background flow, co-authored by M. Dobson, F. Legoll, T. Lelièvre, and G. Stoltz, has been published.

### 5.2.4. *Sampling techniques*

In [29], T. Lelièvre studies with F. Nier and G. Pavliotis (Imperial College, London) the interest of using non-reversible dynamics (overdamped Langevin dynamics with a non-gradient drift term) to efficiently sample a given Boltzmann-Gibbs distribution.

### 5.2.5. *Numerical analysis of simulation methods*

Together with B. Leimkuhler and Ch. Matthews (Edinburgh University), G. Stoltz studied in [48] the discretization errors in the computation of average properties with Langevin dynamics integrated with splitting strategies. The average properties are either static (average of a given observable) or dynamic (transport coefficients). The main tool used in this analysis is the expansion of the transition operator in powers of the time step, with exact integral remainders; as well as fine estimates on the resolvent of the Langevin operators, especially in the so-called overdamped limit where the friction goes to infinity. Transport coefficients are studied either through errors in Green-Kubo formulae or errors in the linear response of nonequilibrium systems.

### 5.2.6. Coarse-graining of molecular systems

G. Stoltz, in collaboration with J.-B. Maillet and G. Faure, developed in [43] a potential energy function depending on the local density of the molecular fluid. The local density is evaluated with a three dimensional Voronoi tessellation, which proves more rigorous than the standard local averages typically found in the literature. The new potential allows to describe the compressibility of mesoparticles representing several molecules in a coarse-grained description of the atomic system. The quality of the potential has been assessed by reproducing equations of state and Hugoniot curves of model energetic materials.

### 5.2.7. Thermodynamic limit

The quasicontinuum method is an approach to couple an atomistic model with a coarse-grained approximation in order to compute the states of a crystalline lattice at a reduced computational cost compared to a full atomistic simulation. In that framework, the team has addressed questions related to the *finite temperature* modeling of atomistic systems and derivation of coarse-grained descriptions, such as canonical averages of observables depending only on a few variables. The work from F. Legoll and X. Blanc (Université Pierre et Marie Curie) is now published [12].

When the temperature is small, a perturbation approach can be used to compute the canonical averages of these observables depending only on a few variables, at first order with respect to temperature. The work from F. Legoll in collaboration with E. Tadmor, W. K. Kim, L. Dupuy and R. Miller on the analysis of such an approach is now also published [32].

### 5.2.8. Hamiltonian dynamics

Constant energy averages are often computed as long time limits of time averages along a typical trajectory of the Hamiltonian dynamics. One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some motions are very high (e.g. for the atomistic bond vibrations), while those of other motions are much smaller. This problem has been addressed in a two-fold manner.

Fast phenomena are often only relevant through their mean effect on the slow phenomena, and their precise description is not needed. The work from M. Dobson, C. Le Bris, and F. Legoll developing integrators for Hamiltonian systems with high frequencies (derived using homogenization techniques applied to the Hamilton-Jacobi PDE associated to the Hamiltonian ODE) is now published [22].

Another track to simulate the system for longer times is to resort to parallel computations. An algorithm in that vein is the parareal in time algorithm. The work from C. Le Bris and F. Legoll, in collaboration with X. Dai and Y. Maday, studying several variants of the original plain parareal in time algorithm, is now also published [21].

### 5.2.9. Effective dynamics

For a given molecular system, and a given reaction coordinate  $\xi : \mathbb{R}^n \mapsto \mathbb{R}$ , the free energy completely describes the statistics of  $\xi(X)$  when  $X \in \mathbb{R}^n$  is distributed according to the Gibbs measure. On the other hand, obtaining a correct description of the dynamics along  $\xi$  is complicated. In this context, S. Lahbabi and F. Legoll have studied in [8] the case when the fine-scale, reference dynamics is a kinetic Monte Carlo model with small and fast time scales, and proved a path-wise convergence to a coarse kinetic Monte Carlo model only retaining slow degrees of freedom.

Another question is how to use a coarse-grained description (involving only the slow degrees of freedom) as a predictor for the dynamics of the actual reference system, involving all degrees of freedom. Together with G. Samaey (KU Leuven), F. Legoll and T. Lelièvre have addressed this question in the parareal framework, and shown in [28] that the precise coupling between both models should be done carefully in order for the algorithm to be efficient. In that case, the algorithm converges to the reference full dynamics.

## 5.3. Complex fluids

**Participants:** David Benoit, Sébastien Boyaval, Claude Le Bris, Tony Lelièvre.

In his PhD under the supervision of Claude Le Bris and Tony Lelièvre, David Benoit studies models of aging fluids developed at the ESPCI (Ecole supérieure de physique et de chimie industrielles) and designed to take into account phenomena such as shear thinning, aging and shear banding in falling sphere experiments. The work consists in studying on the one hand the mathematical well-posedness of some macroscopic models, see [10], and, on the other hand, in trying to understand the link between such macroscopic models and microscopic models which have been proposed to describe such fluids, see [34].

Let us also mention that the paper [28] on a parareal algorithm to efficiently simulate micro-macro models which has been published this year.

Related to the mathematical modelling of free-surface complex flows under gravity, a new reduced model for thin layers of a viscoelastic upper-convected Maxwell fluid was derived by S. Boyaval in collaboration with François Bouchut. Possibly discontinuous solutions were numerically simulated with a new finite-volume scheme of relaxation type that satisfies a discrete counterpart of the natural dissipation [13].

This work has been pursued for other fluid models and other flow regimes, with a view to better understanding the reduction mechanism leading from a physically detailed model to a useful one for numerical simulations at large (geophysical) scales [35].

On the other hand, note that it is often possible to consider only models for *incompressible* fluids (at low Mach numbers). Now, it is both important and delicate to understand how to numerically discretize the incompressibility constraint, a long-standing issue in numerical fluid mechanics. In collaboration with M. Picasso (EPFL), S. Boyaval has thus investigated the possibility to numerically quantify *a posteriori* the quality of a well-known, "simple" numerical method discretizing the incompressibility constraint, in a simple case [36]. This is part of another effort toward useful numerical simulations of complex flows, inline with current questions focused on discretization methods..

## 5.4. Application of greedy algorithms

**Participants:** Sébastien Boyaval, Eric Cancès, Virginie Ehrlicher, Tony Lelièvre.

Model reduction techniques are very important tools for applications. They consist in deriving from a high-dimensional problem, a low-dimensional model, which gives very quickly reliable results. We are in particular interested in two techniques: Proper Generalized Decomposition (greedy algorithms) and Reduced Basis techniques.

Concerning the Proper Generalized Decomposition, current research concerns the approximation of high-dimensional spectral problems, see [38]. Prototypical applications include electronic structure calculations or the computation of buckling modes in mechanics. We also explored in the PhD of J. Infante Acevedo the application of these techniques to option pricing problems, see [45].

Finally, in [40], Fabien Casenave (CERMICS), Alexandre Ern (CERMICS), Guillaume Sylvand (EADS IW) and Tony Lelièvre propose a new non intrusive implementation of the reduced basis technique using the Empirical Interpolation Method. The interest if the method is illustrated on aeroacoustic problems.

## 5.5. Homogenization and related topics

**Participants:** Virginie Ehrlicher, Claude Le Bris, Frédéric Legoll, François Madiot, William Minvielle.

The homogenization of (deterministic) non periodic systems is a well known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc and P.-L. Lions, C. Le Bris has introduced a possible theory, giving rise to a numerical approach, for the simulation of multiscale nonperiodic systems. The theoretical considerations are based on earlier works by the same authors (derivation of an algebra of functions appropriate to formalize a theory of homogenization). The numerical endeavour is completely new. Promising results have been obtained on a simple case of a periodic system perturbed by a localized defect. Ongoing works consider other configurations, such as for instance an interface between two different crystalline phases.

The project-team also has pursued its efforts in the field of stochastic homogenization of elliptic equations, aiming at designing numerical approaches that both are practically relevant and keep the computational workload limited.

Using the standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the *whole* space  $\mathbb{R}^d$ . This equation is therefore delicate and expensive to solve. In practice, the space  $\mathbb{R}^d$  is truncated to some bounded domain, on which the corrector problem is numerically solved. In turn, this yields a converging approximation of the homogenized tensor, which happens to be a *random* matrix. For a given truncation of  $\mathbb{R}^d$ , the team has previously shown that the variance of this matrix can be reduced using the technique of antithetic variables. In [47], F. Legoll and W. Minvielle have extended this technique to nonlinear, convex homogenization problems.

In addition, F. Legoll and W. Minvielle have investigated the possibility to use other variance reduction approaches, such as control variate techniques. A promising idea is to use the weakly stochastic model previously introduced by A. Anantharaman and C. Le Bris (in which a periodic model is perturbed by a *rare* stochastic perturbation) to build a control variate model. The preliminary results that have already been obtained are very encouraging.

Yet another approach to reduce the variance is the so-called Multi Level Monte Carlo (MLMC) approach, which is based on using a surrogate model for the quantity of interest. The MLMC approach consists in using many realizations of the surrogate model (which is cheap to evaluate) and few realizations of the reference model (which is more expensive to evaluate). In collaboration with Y. Efendiev and C. Kronsbein, F. Legoll has explored in [41] how this approach can be used in random homogenization.

We have discussed above approaches to efficiently compute the homogenized coefficient, assuming we have a complete knowledge of the microstructure of the material. We have recently started to consider a related inverse problem, and more precisely a parameter fitting problem. Knowing the homogenized quantities, is it possible to recover some features of the microstructure properties? Obviously, since homogenization is an averaging procedure, not everything can be recovered from macroscopic quantities. A realistic situation is the case when we assume a functional form of the distribution of the microscopic properties, but with some unknown parameters that we would like to determine. In collaboration with A. Obliger and M. Simon, F. Legoll and W. Minvielle have started to address that problem, determining the unknown parameters of the microscopic distribution on the basis of macroscopic (e.g. homogenized) quantities. The preliminary results that have been obtained are very encouraging.

From a numerical perspective, the Multiscale Finite Element Method (MsFEM) is a classical strategy to address the situation when the homogenized problem is not known (e.g. in difficult nonlinear cases), or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as an accurate enough approximation).

The MsFEM has been introduced more than 10 years ago. However, even in simple deterministic cases, there is actually still room for improvement in many different directions. In collaboration with A. Lozinski (University of Besançon), F. Legoll and C. Le Bris have introduced and studied a variant of MsFEM that considers Crouzeix-Raviart type elements on each mesh element. The continuity across edges (or facets) of the (multiscale) finite element basis set functions is enforced only weakly, using fluxes rather than point values. The approach has been analyzed (combining classical arguments from homogenization theory and finite element theory) and tested on simple, but highly convincing cases [27]. In particular, an elliptic problem set on a domain with a huge number of perforations has been considered in [37]. The variant developed outperforms all existing variants of MsFEM.

A follow up on this work, in collaboration with U. Hetmaniuk (University of Washington in Seattle) and A. Lozinski (University of Besançon), consists in the study of multiscale advection-diffusion problems. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interferes with the multiscale character of the equation is an unsolved mathematical question

worth considering for numerical purposes. This is the aim of the PhD thesis of François Madiot, which began in October 2013.

Still another question related to homogenization theory that is investigated in the group is the following. Consider an elliptic equation, say in divergence form, with a highly oscillatory matrix coefficient. Is it possible to approximate the boundary value problem for different right hand sides using a similar problem with a *constant* matrix coefficient? How can this “best” constant matrix approximating the oscillatory problem be constructed in an efficient manner? We have addressed some of these questions in [25], where we have in particular shown that this best constant matrix converges to the homogenized matrix, in the limit of infinitely rapidly oscillatory coefficients. Our approach can therefore be considered as an alternative way to compute the homogenized matrix. This is particularly interesting in random cases, where the standard approach is very expensive. Current work is directed towards extending the approach, in order to compute other quantities of interest than the homogenized coefficient.

To conclude this section, we mention the project undertaken by V. Ehrlacher during her six months postdoctoral position in the Cluster of Excellence Engineering of Advanced Materials (Erlangen University). This project, in collaboration with C. Le Bris, F. Legoll, G. Leugering and M. Stingl, aims at optimizing the shape of some materials (modelled as structurally graded linear elastic materials) in order to achieve the best mechanical response at the minimal cost. As often the case in shape optimization, the solution tends to be highly oscillatory, thus the need of homogenization techniques. We thus consider an initial microstructured material composed of steel and void and whose microstructure pattern is periodic (think e.g. of a periodic honeycomb structure). We next consider materials which are obtained from this initial material through a macroscopic deformation, and look for the optimal deformation achieving the best mechanical response. Encouraging first results have been obtained.

## 5.6. Coupling methods and variance reduction

**Participant:** Mathias Rousset.

Recently, M. Rousset has initiated a research topic on variance reduction techniques (called “asymptotic”) for the simulation of stochastic models of particles. The point is to use a macroscopic (or model reduced) equation as a control variate; or in other words, to use the information of a macroscopic description to decrease the statistical error of the simulated microscopic evolution.

A first step in this program has been achieved for a microscopic model describing the individual motion of bacteriae with a Markovian velocity-jump process. The macroscopic equation is an advection-diffusion equation called the chemotaxis equation. In [30], the probabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out in a rigorous way. In [31], a numerical method simulating the individual evolution of bacteriae with “asymptotic” variance reduction have been proposed.

Motivated by the asymptotic variance reduction of DSMC methods (particle Monte-Carlo methods simulating low density fluids modeled by kinetic equations), the work in [50], M. Rousset considers space homogenous Boltzmann kinetic equations in dimension  $d$  with Maxwell collisions (and without Grad’s cut-off). An explicit Markov coupling of the associated conservative (Nanbu) stochastic  $N$ -particle system is constructed, using plain parallel coupling of isotropic random walks on the sphere of two-body collisional directions. The resulting coupling is almost surely decreasing, and the  $L_2$ -coupling creation is computed explicitly. Some quasi-contractive and uniform in  $N$  coupling / coupling creation inequalities are then proved, relying on  $2 + \alpha$ -moments ( $\alpha > 0$ ) of velocity distributions; upon  $N$ -uniform propagation of moments of the particle system, it yields a  $N$ -scalable  $\alpha$ -power law trend to equilibrium. The latter are based on an original sharp inequality, which bounds from above the coupling distance of two centered and normalized random variables  $(U, V) \in \mathbb{R}^d$ , with the average square parallelogram area spanned by  $(U - U_*, V - V_*)$ ,  $(U_*, V_*)$  denoting an independent copy. Two counter-examples proving the necessity of the dependance on  $> 2$ -moments and the impossibility of strict contractivity are provided. The paper, (mostly) self-contained, does not require any propagation of chaos property and uses only elementary tools.



## 6. Bilateral Contracts and Grants with Industry

### 6.1. Contracts and Grants with Industry

Many research activities of the project-team are conducted in close collaboration with private or public companies: CEA, SANOFI, Safety Line, ERAMET, IRDEP, EADS . The project-team is also supported by Office of Naval Research and European Office of Aerospace Research and Development, for multiscale simulations of random materials. All these contracts are operated at and administrated by the Ecole des Ponts.

### 6.2. National Initiatives

The project-team is involved in several ANR projects:

- the ANR MANIF focuses on the mathematical and numerical analysis of electronic structure models, such as, in particular, the Kohn-Sham model. It includes two research teams: researchers from the JL Lions Laboratory (Paris 6) and the Micmac team. It is coordinated by E. Cancès.
- E. Cancès is involved in the ANR BECASIM, which is concerned with the numerical simulation of Bose-Einstein condensates. This ANR has been accepted in June 2012, and is coordinated by I. Danaila (Université de Rouen).
- C. Le Bris participates to the ANR EMAQS. The scientist in charge is Karine Beauchard (CMLS, Ecole polytechnique).
- T. Lelièvre is member of the ANR-project "STAB" (PI: I. Gentil, Université de Lyon).

In addition, the team is participating in

- the GdR Quantum dynamics. This interdisciplinary research network is focused on physical and mathematical problems related to the time evolution of quantum systems (transport problems, nonequilibrium systems, etc),
- the GdR CoDFT,
- the GdR Maths et entreprise,
- the GdR correl (correlated methods in electronic structure computations),
- the GDR-CNRS 2434 Analyse des Equations aux Dérivées Partielles.

The MICMAC team project is involved in two Labex, namely the Labex Bezout (started in 2011) and the Labex MMCD (started in 2012).

We have invited the following National researchers to visit our team:

- A. Lozinski (University of Besançon): April 8-12 and Dec 16-20, 2013.

## 7. Partnerships and Cooperations

### 7.1. International Initiatives

T. Lelièvre, G. Stoltz and F. Legoll participate to the Laboratoire International Associé (LIA) CNRS / University of Illinois at Urbana-Champaign on complex biological systems and their simulation by high performance computers. This LIA involves on the french side research teams from Université Nancy, Université de Lyon and Inria Rennes.

### 7.2. International Research Visitors

#### 7.2.1. Visits of International Scientists

We have invited the following researchers to visit our team:

- U. Hetmaniuk (University of Washington in Seattle), April 8-12, 2013, and Dec 16-20, 2013.



## 8. Dissemination

### 8.1. Animation of the scientific community

S. Boyaval has co-organized:

- at SMAI 2013, Seignosse, 2 minisymposiums: "écoulements complexes en rivières" with E. Audusse and "Interactions Fluide-Structure" with M. Fernandez and L. Monasse.

E. Cancès

- is a member of the editorial boards of Mathematical Modelling and Numerical Analysis (2006-), of SIAM Journal of Scientific Computing (2008-), of Communications in Mathematical Sciences (2011-),
- is a member of the executive committee of the CEA-EDF-Inria schools in applied mathematics and computer science,
- is a member of the scientific committee of the GDR co-DFT.

He has organized or co-organized:

- the SIAM MS Minisymposium on "Electronic structure calculation", Philadelphia, USA, June 2013,
- the IHP mini-workshop on "The mathematics of interacting quantum systems in a random environment", Paris, June 2013,

C. Le Bris is editor-in-chief of Applied Mathematics Research Express (2003-). He is a member of the editorial boards of Annales mathématiques du Québec (2013-), Archive for Rational Mechanics and Analysis (2004-), COCV (Control, Optimization and Calculus of Variations) (2003-), Mathematics in Action (2008-), Networks and Heterogeneous Media (2005-), Nonlinearity (2005-), Journal de Mathématiques Pures et Appliquées (2009-).

He is a member of the editorial boards of the monograph series Mathématiques & Applications, Series, Springer (2008-), and Modeling, Simulations and Applications, Series, Springer (2009-).

C. Le Bris is a member of

- the Cabinet of the High Commissioner for Atomic Energy,
- the scientific board of ENPC, 2008- (nominated as representative of the research scholars),
- the "Comité d'experts" for the "Fondation de Recherche pour l'Aéronautique et l'Espace",
- the "Comité d'animation du domaine thématique Mathématiques appliquées, calcul et simulation" at Inria,
- the "International Scientific Advisory Committee" of the Centre de Recherche Mathématique, Université de Montréal,
- the "Advisory Board" of the DFG Cluster of Excellence Engineering of Advanced Materials, Erlangen,
- the "International Scientific Advisory Board" of the DFG research center Matheon, Berlin,
- the "Conseil de perfectionnement du Master de Mathématiques" of the University Pierre et Marie Curie.

C. Le Bris has held a position of Visiting Professor at the University of Chicago, February-October-November 2013.

He has been a member of

- the Organizing Committee of the SIAM Materials Science meeting, 2013.
- the Scientific Committee of CANUM 2014.

He has co-organized

- with G. Bal, B. Engquist, H. Owhadi, the Oberwolfach workshop *Interplay of theory and numerics for deterministic and stochastic Homogenization*, Oberwolfach, 17-23 March 2013,
- with Ch. Lubich, the workshop *Mathematical and numerical challenges in quantum chemistry*, Institut Henri Poincaré, Paris, June 2013,
- with P.-M. Mariano, the one-week school *Multi-scale and multi-field representations of condensed matter behavior* at the Centro De Giorgi, Pisa, Italy, 25-29 November 2013,
- with S. Adams, J. Ball, Ch. Ortner, the workshop *Computational coarse graining of many-body systems*, University of Warwick, 9-13 December 2013.

F. Legoll

- is a member of the editorial board of SIAM MMS (2012-) and of ESAIM Proc (2012-),
- has co-organized with Y. Maday a mini-symposium on "Recent advances on parareal algorithms" at the SciCADE 2013 conference, Valladolid, September 16-20, 2013,
- has co-organized with R. Cottreau, L. Graham-Brady and M. Ostojca-Starzewski a mini-symposium on "Multi-scale methods for heterogeneous materials" at the 12th U.S. National Congress on Computational Mechanics (12th USNCCM), Raleigh, July 22-25, 2013,
- has co-organized with B. Kraczek, R. Jones and K. Mandadapu a mini-symposium on "The atomistic basis of non-equilibrium thermal processes in materials" at the 12th U.S. National Congress on Computational Mechanics (12th USNCCM), Raleigh, July 22-25, 2013.

T. Lelièvre

- is editor-in-chief of ESAIM: Proceedings (with D. Chafai, P. Lafitte and C. Mouhot).
- was an Ordway visiting professor at the University of Minnesota for the academic year 2012-2013 (one month-stay in April 2013).
- has co-organized the CEMRACS 2013 summer school: "Modelling and simulation of complex systems: stochastic and deterministic approaches" (with N. Champagnat and A. Nouy).
- has co-organized the workshop NASPDE (Numerical Analysis of Stochastic PDEs), 10 and 11 September 2013 (with E. Faou and J. Erhel).
- co-organizes the Journées EDP-Probab at Institut Henri Poincaré (with F. Malrieu).
- is the head of the GDR MoMaS, a French research group on the mathematical modeling and the numerical simulations for nuclear waste management problems (Main scientific themes: multiscale models for flows in porous media, molecular simulation of clays, multiphase flows).
- is in charge of the Theme 4 (Stochastic modeling, quantification and uncertainty propagation for multiscale mechanical models of materials) of the Labex MMCD.

## 8.2. Teaching - Supervision

The members of the team have taught the following courses:

- Licence: Calcul Scientifique, 12h, L3, Ecole des Ponts ParisTech (S. Boyaval).
- Licence: probabilités deuxième semestre, 12h, Ecole Centrale de Paris, (S. Boyaval).
- Licence: Analyse, 36h, L3, Ecole des Ponts, France (E. Cancès, F. Legoll, G. Stoltz, M. Rousset, W. Minvielle, V. Ehrlacher)
- Licence : Fonctions à plusieurs variables et équations différentielles, 60h, L2, ESIEE, France (D. Gontier)
- Licence: Projets de physique, 20h, L3, Ecole des Ponts, France (I. Dabo, G. Stoltz)
- Master: Processus Stochastiques, 18h. M1, ESIEA (C.-E. Bréhier).
- Master: Analyse spectrale, 39h, M1, Ecole des Ponts, France (G. Stoltz, V. Ehrlacher)

- Master: Méthodes déterministes en mathématiques financières, 42h, M2, Ecole des Ponts ParisTech (T. Lelièvre).
- Master: Modéliser Programmer Simuler, 28 h, M1, Cours Ecole des Ponts ParisTech (T. Lelièvre).
- Master: Méthodes numériques probabilistes, 36 h, M2 Mathématiques et Applications, Université Pierre et Marie Curie (T. Lelièvre).
- Master: Mathématiques des modèles multiéchelles, 39h, M1, Ecole des Ponts ParisTech, France (F. Legoll)
- Master: Problèmes multi-échelles, 24h, M2, Université Paris 6, France (F. Legoll)
- Master: Introduction au calcul Scientifique, 12h, M1, Ecole des Mines ParisTech, France (D. Benoit, W. Minvielle, G. Stoltz, F. Madiot)
- Master: Analyse Numérique et Optimisation, 56h, M1, Ecole Polytechnique, France (E. Cancès)
- Master: Méthodes variationnelles en mécanique quantique, 12h, M2, University Paris 6, France (E. Cancès)
- Master: Analyse spectrale, 39h, M1, Ecole des Ponts, France (V. Ehrlacher, G. Stoltz)
- Master: Spectral theory of Schrodinger operators, 30h, M2, Université de Marne-la-Vallée, France (G. Stoltz)
- Master: Outils Probabilistes pour la Finance, 24h, M1, Cours Ecole des Ponts ParisTech (M. Rousset).

The following PhD were defended by students members of the research group at the Ecole des Ponts:

- I. Acevedo Méthodes et modèles numériques appliqués aux risques du marché et à l'évaluation financière, Université Paris-Est, Université Paris Est, 10 dec. 2013, supervised by A. Alfonsi (Ecole des Ponts) et T. Lelièvre.
- F. Casenave, Méthodes de réduction de modèles appliquées à des problèmes d'aéroacoustique résolus par équations intégrales, Université Paris-Est, Université Paris Est, 10 dec. 2013, supervised by A. Ern (Ecole des Ponts) et T. Lelièvre.
- S. Lahbabi, Etude mathématique de modèles quantiques et classiques pour les matériaux aléatoires à l'échelle atomique, Université de Cergy Pontoise, supervised by E. Cancès and M. Lewin, July 2013.

The following PhDs are in progress:

- D. Benoit, Méthodes numériques pour la simulation des fluides non-Newtoniens, Université Paris-Est, Université Paris Est, started October 1st, 2010, supervised by C. Le Bris and T. Lelièvre, to be defended on January 22nd 2014.
- F. Madiot, Multiscale finite element methods for advection diffusion problems, Université Paris-Est, Ecole des Ponts ParisTech, started october 1st, 2013, supervised by C. Le Bris and F. Legoll
- W. Minvielle, Méthodes numériques pour les matériaux, Université Paris-Est, Université Paris Est, started october 1st, 2012, supervised by C. Le Bris and F. Legoll
- D. Gontier, Université Paris-Est, started September 1st, 2012, supervised by E. Cancès
- A.-A. Homman, Multiscale methods for the simulation of shock and detonation waves, Université Paris-Est, Ecole des Ponts ParisTech and CEA/DAM, started April 1st, 2013, supervised by G. Stoltz and J.-B. Maillet

### 8.3. Conference participation

Members of the project-team have delivered lectures in the following seminars, workshops and international conferences:

- S. Boyaval, NASCA 2013 (Calais)
- S. Boyaval, CEMRACS 2013
- S. Boyaval, seminar at the Universities of Montpellier and Toulouse
- C.-E. Bréhier, Conference NASPDE 2013, Rennes, September 2013.
- E. Cancès, workshop on Mathematical and numerical methods for electronic structure calculation, Berlin, January 2013.
- E. Cancès, workshop on Multiscale modeling, analysis, and computation of nano-optics, Michigan State University, Lansing, USA, March 2013.
- E. Cancès, IMA workshop on Mathematics and Chemistry, Chicago, April 2013.
- E. Cancès, Weekly seminar, Mathematics department, University of Chicago, USA, May 2013.
- E. Cancès, SIAM MS 2013, Philadelphia, USA, June 2013.
- E. Cancès, IHP mini-workshop on Mathematical and numerical challenges in quantum chemistry, Paris, June 2013.
- E. Cancès, plenary lecture, Enumath 2013, Lausanne, August 2013.
- E. Cancès, Enumath minisymposium on Multiscale methods for atomistic and continuum problems, Lausanne, August 2013.
- E. Cancès, IPAM workshop on Semiclassical origins of Density Functional Approximations, Los Angeles, September 2013.
- E. Cancès, plenary lecture, Q-Math 12, Berlin, September 2013.
- E. Cancès, IPAM workshop on Fuels from sunlight, Los Angeles, October 2013.
- E. Cancès, Conference in honor of Wolfgang Hackbusch's 65th birthday, Leipzig, October 2013.
- V. Ehrlacher, SIAM Conference on Computational Science and Engineering (CSE13), Boston, USA, February 2013.
- V. Ehrlacher, Seminar Zentrum Mathematik, TU München, Munich, Germany, February 2013.
- V. Ehrlacher, Applied mathematics seminar of Warwick University, Warwick, England, February 2013.
- V. Ehrlacher, Oberwolfach workshop on Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization, Oberwolfach, Germany, February 2013.
- V. Ehrlacher, Congrès SMAI 2013, Seignosse, France, May 2013.
- V. Ehrlacher, CIRM workshop on Model Reduction and Approximation for Complex Systems, Luminy, France, June 2013.
- V. Ehrlacher, Seminar of Excellence cluster of Engineering of Advanced Materials, Erlangen, Germany, June 2013.
- V. Ehrlacher, Mathematik Seminar der Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, June 2013.
- V. Ehrlacher, CEMRACS 2013, CIRM, Luminy, France, August 2013.
- V. Ehrlacher, ENUMATH, Lausanne, Switzerland, August 2013.
- V. Ehrlacher, QMATH 12, workshop on Mathematical results in quantum mechanics, Berlin, Germany, September 2013.
- V. Ehrlacher, Séminaire du laboratoire GeM, Ecole centrale Nantes, France, September 2013.

- V. Ehrlacher, Séminaire du laboratoire Jacques-Louis Lions, Université Paris 6, France, November 2013.
- V. Ehrlacher, MATHICSE seminar, EPFL, Lausanne, Switzerland, December 2013.
- D. Gontier, Annual meeting of the GDR co-DFT, Guidel, France, May 2013.
- D. Gontier, IHP Seminar, Paris, July 2013.
- S. Lahbabi, weekly seminar of the mathematics department University of Pau, May 2013.
- S. Lahbabi, IHP workshop on Mathematical properties of large quantum systems, Paris, June 2013.
- C. Le Bris, plenary lecture, SMAI 2013, Seignosse, 27-31 May 2013
- C. Le Bris, Workshop "Numerical Methods for Uncertainty Quantification", May 13-17, 2013, Hausdorff Center for Mathematics, Bonn.
- C. Le Bris, SIAM Materials Modeling minisymposium, Philadelphia, June 9-12, 2013.
- C. Le Bris, 2nd Pacific Rim Mathematical Association Congress, Shanghai, June 24-28, 2013.
- C. Le Bris, Scientific and statistical computing seminar University of Chicago
- C. Le Bris, Argonne National Laboratory,
- C. Le Bris, Colloquium of the Max Planck Institute Leipzig,
- C. Le Bris, Colloquium Ecole Polytechnique Fédérale de Lausanne,
- C. Le Bris, Computations in Science Seminar of the university of Chicago,
- C. Le Bris, PDE Seminar of the university of Chicago,
- C. Le Bris, Inaugural lecture in Mathematics for the "Semaine de la Science", Ecole Polytechnique
- F. Legoll, weekly seminar of the mathematics department, Université de Besançon, February 2013
- F. Legoll, weekly seminar of the Jacques-Louis Lions laboratory, March 2013
- F. Legoll, workshop on Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization, Oberwolfach, March 2013
- F. Legoll, workshop on multiscale modelling and simulation in material science, Shanghai, April 2013
- F. Legoll, 11ieme Colloque National en Calcul des Structures, Giens, May 2013
- F. Legoll, workshop on slow-fast dynamics, Barcelona, June 2013
- F. Legoll, SIAM conference on mathematical aspects of material sciences, Philadelphia, June 2013
- F. Legoll, 12th US National Congress on Computational Mechanics, Raleigh, July 2013
- F. Legoll, SES 50th Annual Technical Meeting, Providence, July 2013
- F. Legoll, CEMRACS summer school, Marseille, August 2013
- F. Legoll, SciCADE conference, Valladolid, September 2013
- F. Legoll, MoMaS Multiphase Seminar Days, Orsay, October 2013
- F. Legoll, workshop "Stochastic Modeling of Multiscale Systems", Eindhoven, december 2013
- F. Legoll, Symposium on Statistical Mechanics, Warwick, december 2013
- T. Lelièvre, Kolloquium, Institut für Mathematik, Universität Mainz, January 2013.
- T. Lelièvre, Séminaire ANR BIGMC, Paris, February 2013.
- T. Lelièvre, Séminaire Institut de Mathématiques de Toulouse, March 2013.
- T. Lelièvre, Workshop "Genetic models and Quasi-stationarity", CIRM, Marseille, March 2013.
- T. Lelièvre, Workshop "Analysis and Stochastics in Complex Physical Systems", Leipzig, March 2013.
- T. Lelièvre, Math colloquium, University of Minnesota, April 2013.
- T. Lelièvre, PDE seminar, University of Minnesota, April 2013.

- T. Lelièvre, Workshop Randomness and PDE, Labex Lebesgue semester, Nantes, April 2013.
- T. Lelièvre, IMA Chem year Summit, Chicago, May 2013.
- T. Lelièvre, SMAI 2013, May 2013.
- T. Lelièvre, Plenary speaker at the SIAM conference on Mathematical Aspects of Materials Science, Philadelphia, June 2013.
- T. Lelièvre, Workshop Scicade 2013, Valladolid, September 2013.
- T. Lelièvre, Workshop on Reduced Basis, POD and PGD model, Blois, November 2013.
- T. Lelièvre, Séminaire de la Chaire FDD, IHP, Paris, December 2013.
- T. Lelièvre, Workshop “Computational coarse-graining of many-body systems”, Warwick, December 2013.
- T. Lelièvre, Workshop on Material Theories, Oberwolfach, December 2013.
- F. Nier, Collège de France, April 2013,
- F. Nier, workshop of the ANR Lodiquas à Vienne (Autriche), July 2013: Artificial gauge and adiabatic Ansatz for Bose-Einstein condensates.
- F. Nier, Berkeley, September 2013,
- F. Nier, Institute for Pure and Applied Mathematics, Workshop “Semiclassical Origins of Density Functional Theory”, Los Angeles, September 2013,
- F. Nier, CIRM, Microlocal analysis and spectral theory, September 2013,
- F. Nier, Orsay, Working group “Opérateurs de Dirac”, December 2013,
- M. Rousset, SIAM conference on mathematical aspects of material sciences, Philadelphia, June 2013
- M. Rousset, CEMRACS summer school, Marseille, August 2013.
- M. Rousset, Séminaire Institut de Mathématiques de Toulouse (Probabilités), December 2013
- G. Stoltz, Oberwolfach meeting "Large Scale Stochastic Dynamics" (Germany), October 2013
- G. Stoltz, QMaths12, Berlin (Germany), September 2013
- G. Stoltz, GDRE ConEDP Meeting, Grenoble (France), April 2013
- G. Stoltz, AMMP seminar, Imperial College London (United-Kingdom), October 2013
- G. Stoltz, daily seminar at CEMRACS 2013, Marseille (France), August 2013
- G. Stoltz, Mathematical Physics Seminar, Institut Poincaré, Paris (France), May 2013

In addition to the above, some members of the team have been invited for stays in institutions abroad:

- E. Cancès, University of Chicago, April-May 2013,
- E. Cancès, IPAM, UCLA, October 2013,
- T. Lelièvre, one month at the University of Minnesota as an Ordway professor.

Members of the project-team have delivered the following series of lectures:

- E. Cancès (15h) on numerical methods for electronic structure calculation, Summer school on the scientific trends at the interfaces mathematics - chemistry - high performance computing, Roscoff, France, July-August 2013,
- E. Cancès (6h) on the mathematics of quantum chemistry, Oberwolfach seminar, Germany, November 2013,
- C. Le Bris, Lectures on ‘Numerical homogenization’, The University of Chicago, 12 hours, February 2013,
- C. Le Bris, Lectures on ‘Renormalized solutions to parabolic equations’, The University of Chicago, 20 hours, Fall 2013,

- C. Le Bris, Lectures on 'Stochastic homogenization and related problems', Series of 4 one-hour lectures, Multi-scale and Multi-field Representations of Condensed Matter Behavior, Scuola Normale Pisa, November 2013,
- T. Lelièvre, Lectures on the adaptive biasing force method at the University of Minnesota,
- G. Stoltz, Lectures (4h) on "Molecular simulation: A mathematical introduction", School "Multi-scale and Multi-field Representations of Condensed Matter Behavior", Pisa (Italy), November 2013
- G. Stoltz, Lectures (4h) on "Molecular simulation: A mathematical introduction", School "Longtime limits of stochastic models" at CIRM, Marseille (France), February 2013
- G. Stoltz (9h) on numerical methods for statistical physics, Summer school on the scientific trends at the interfaces mathematics - chemistry - high performance computing, Roscoff, France, July-August 2013.

Members of the project-team have participated (without giving talks nor presenting posters) in the following seminars, workshops and international conferences:

- D. Gontier, Q-Math 12, Berlin, September 2013.
- D. Gontier, Oberwolfach seminar, November 2013.
- W. Minvielle, "Ecole Thématique du GdR CHANT", January 2013
- W. Minvielle, workshop on Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization, Oberwolfach, March 2013
- W. Minvielle, Summer School in Analysis and Applied Mathematics, Roma, June 2013
- W. Minvielle, CEMRACS summer school, Marseille, August 2013
- W. Minvielle, workshop on "Quasistatic and Dynamic Evolution Problems in Plasticity and Fracture", Trieste, October 2013

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- [4] J.-F. GERBEAU, C. LE BRIS, T. LELIÈVRE. , *Mathematical Methods for the Magnetohydrodynamics of Liquid Metals*, Numerical Mathematics and Scientific Computation. Oxford: Oxford University Press., 324 p., 2006
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- [6] T. LELIÈVRE, M. ROUSSET, G. STOLTZ. , *Free Energy Computations: A Mathematical Perspective*, Imperial College Press, 458 p., 2010

## Publications of the year

### Doctoral Dissertations and Habilitation Theses

- [7] J. A. INFANTE ACEVEDO. , *Méthodes et modèles numériques appliqués aux risques du marché et à l'évaluation financière*, Université Paris-Est, December 2013, <http://hal.inria.fr/tel-00937131>
- [8] S. LAHBABI. , *Etude mathématique de modèles quantiques et classiques pour les matériaux aléatoires à l'échelle atomique*, Université de Cergy Pontoise, July 2013, <http://hal.inria.fr/tel-00873213>

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- [10] D. BENOIT, L. HE, C. LE BRIS, T. LELIÈVRE. *Mathematical analysis of a one-dimensional model for an aging fluid*, in "Mathematical Models and Methods in Applied Sciences", August 2013, pp. 1561-1602 [DOI : 10.1142/S0218202513500164], <http://hal.inria.fr/hal-00676678>
- [11] X. BLANC, F. LEGOLL, A. ANANTHARAMAN. *Asymptotic behaviour of Green functions of divergence form operators with periodic coefficients*, in "Applied Mathematics Research eXpress", 2013, vol. 2013, n<sup>o</sup> 1, pp. 79-101, <http://hal.inria.fr/hal-00637489>
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